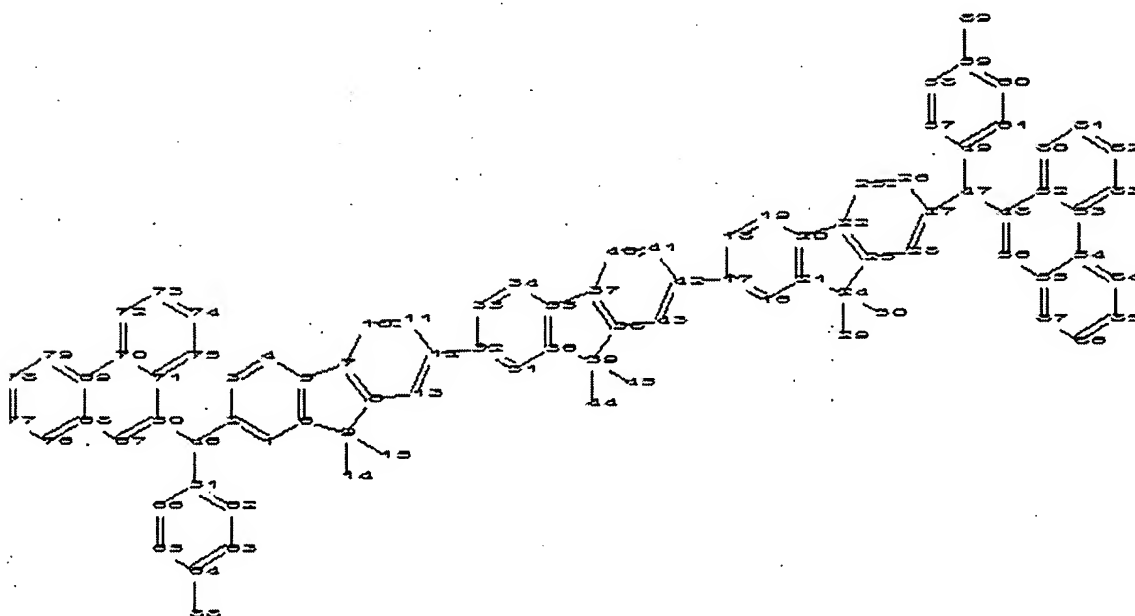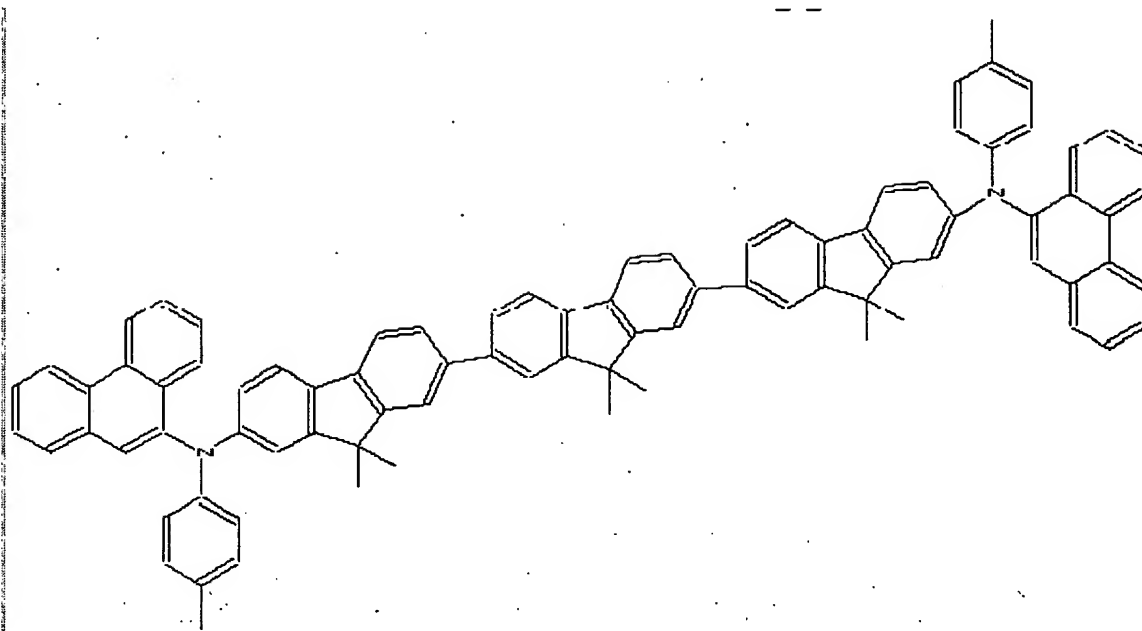=> file reg

chain nodes :
14 15 29 30 44 45 46 47 88 89
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 16 17 18 19 20 21 22 23 24 25

26 27 28 31 32 33 34 35 36 37 38 39 40 41 42 43 48 49 50 51 52 53 54 55
56
57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80
81 82 83 84 85 86 87
chain bonds :
2-46 9-14 9-15 12-32 17-42 24-29 24-30 27-47 39-44 39-45 46-50 46-51
47-48 47-49 59-89 64-88
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 7-10 8-9 8-13 10-11 11-12 12-13
16-17 16-21 17-18 18-19 19-20 20-21 20-22 21-24 22-23 22-25 23-24 23-28 25-
26 26-27
27-28 31-32 31-36 32-33 33-34 34-35 35-36 35-37 36-39 37-38 37-40 38-39 38-
43 40-41
41-42 42-43 48-52 48-56 49-57 49-61 50-67 50-71 51-62 51-66 52-53 52-80 53-
54 53-83 54-55
54-84 55-56 55-87 57-58 58-59 59-60 60-61 62-63 63-64 64-65 65-66 67-68 68-
69 68-76
69-70 69-79 70-71 70-72 71-75 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-
82 82-83
84-85 85-86 86-87
exact/norm bonds :
2-46 5-7 6-9 8-9 20-22 21-24 23-24 27-47 35-37 36-39 38-39 46-50 46-51
47-48 47-49
exact bonds :
9-14 9-15 12-32 17-42 24-29 24-30 39-44 39-45 59-89 64-88
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-10 8-13 10-11 11-12 12-13 16-17 16-21
17-18 18-19 19-20 20-21 22-23 22-25 23-28 25-26 26-27 27-28 31-32 31-36 32-
33 33-34
34-35 35-36 37-38 37-40 38-43 40-41 41-42 42-43 48-52 48-56 49-57 49-61 50-
67 50-71 51-62
51-66 52-53 52-80 53-54 53-83 54-55 54-84 55-56 55-87 57-58 58-59 59-60 60-
61 62-63
63-64 64-65 65-66 67-68 68-69 68-76 69-70 69-79 70-71 70-72 71-75 72-73 73-
74 74-75
76-77 77-78 78-79 80-81 81-82 82-83 84-85 85-86 86-87

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom
19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS
30:CLASS 31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom
41:Atom 42:Atom 43:Atom

44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:Atom .
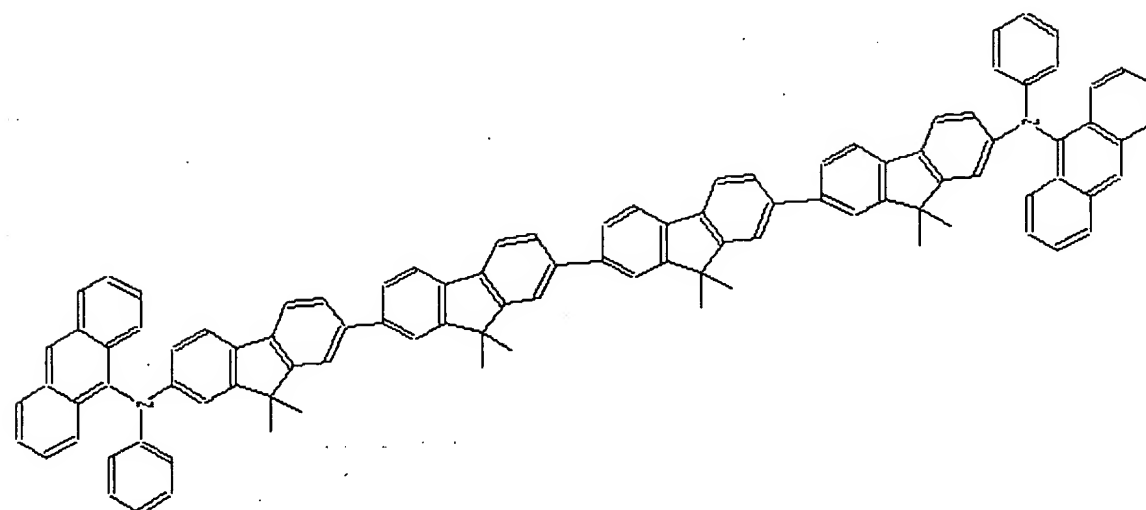88:CLASS 89:CLASS

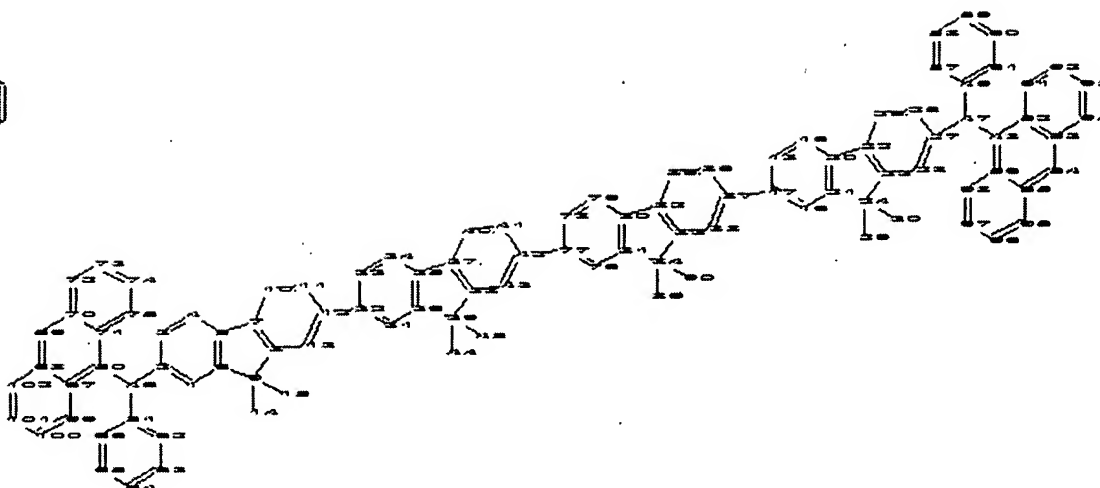L1   STRUCTURE UPLOADED

=> s l1 sss ful

L3   1 SEA SSS FUL L1

=> file hcaplus

=> s l3
L4   1 L3

=> file reg

chain nodes :

14 15 29 30 44 45 46 47 89 90

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 16 17 18 19 20 21 22 23 24 25
26 27 28 31 32 33 34 35 36 37 38 39 40 41 42 43 48 49 50 51 52 53 54 55 56
57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80
81 82 83 84 85 86 87 88 91 92 93 94 95 96 97 98 99 100 101 102

chain bonds :

2-46 9-14 9-15 12-32 17-87 24-29 24-30 27-47 39-44 39-45 42-77 46-50
46-51 47-48 47-49 84-89 84-90

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 7-10 8-9 8-13 10-11 11-12 12-13
16-17 16-21 17-18 18-19 19-20 20-21 20-22 21-24 22-23 22-25 23-24 23-28 25-26 26-27
27-28 31-32 31-36 32-33 33-34 34-35 35-36 35-37 36-39 37-38 37-40 38-39 38-43 40-41
41-42 42-43 48-52 48-56 49-57 49-61 50-67 50-71 51-62 51-66 52-53 52-91 53-54 53-94 54-55
55-56 55-95 56-98 57-58 58-59 59-60 60-61 62-63 63-64 64-65 65-66 67-68 67-99 68-69
68-102 69-70 70-71 70-72 71-75 72-73 73-74 74-75 76-77 76-81 77-78 78-79 79-80 80-81
80-82 81-84 82-83 82-85 83-84 83-88 85-86 86-87 87-88 91-92 92-93 93-94 95-96 96-97
97-98 99-100 100-101 101-102

exact/norm bonds :

2-46 5-7 6-9 8-9 20-22 21-24 23-24 27-47 35-37 36-39 38-39 46-50 46-51
47-48 47-49 80-82 81-84 83-84

exact bonds :

9-14 9-15 12-32 17-87 24-29 24-30 39-44 39-45 42-77 84-89 84-90
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-10 8-13 10-11 11-12 12-13 16-17 16-21
17-18 18-19 19-20 20-21 22-23 22-25 23-28 25-26 26-27 27-28 31-32 31-36 32-
33 33-34
34-35 35-36 37-38 37-40 38-43 40-41 41-42 42-43 48-52 48-56 49-57 49-61 50-
67 50-71 51-62
51-66 52-53 52-91 53-54 53-94 54-55 55-56 55-95 56-98 57-58 58-59 59-60 60-
61 62-63
63-64 64-65 65-66 67-68 67-99 68-69 68-102 69-70 70-71 70-72 71-75 72-73 73-
74 74-75
76-77 76-81 77-78 78-79 79-80 80-81 82-83 82-85 83-88 85-86 86-87 87-88 91-
92 92-93
93-94 95-96 96-97 97-98 99-100 100-101 101-102

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom
19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS
30:CLASS 31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom
41:Atom 42:Atom 43:Atom
44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:Atom 49:Atom 50:Atom 51:Atom
52:Atom 53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom
63:Atom 64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom
74:Atom 75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:Atom
88:Atom 89:CLASS 90:CLASS 91:Atom 92:Atom 93:Atom 94:Atom 95:Atom
96:Atom 97:Atom
98:Atom 99:Atom 100:Atom 101:Atom 102:Atom

L5   STRUCTURE UPLOADED

=> s l5 sss ful

L7   1 SEA SSS FUL L5

=> file hcaplus

=> s l7
L8   1 L7